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Statistical Model for Mechanical Failure

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ABSTRACT

We study a statistical mechanics model of a solid subjected to stress and temperature. In this model the pair energy of a "spring" is given by the universal energy-lattice constant relationship developed by Ferrante et al. If the energy is larger than a threshold the "spring" fails. Two different mechanisms for mechanical failure are identified: (1) the solid becomes soft when the isothermal derivative of stress with respect to strain vanishes; (2) the solid crumbles when the net of failed "springs" percolates. The phase diagram is determined in the temperature, stress plane exhibiting the locus of points where the solid becomes soft and where it crumbles. The phase diagram is universal when the temperature and stress are appropriately scaled.

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I. INTRODUCTION

The mechanical properties of solids, such as the mechanical failure, are topics of considerable current interest (refs. 1 to 3) for both practical and fundamental reasons. In this paper we analyze an equilibrium statistical mechanics model (refs. 4 and 5) of a solid. In our calculations we go beyond the ideal Hooke law for springs by using the realistic anharmonic energy versus atomic distance developed and tested extensively by Ferrante and his collaborators (ref. 6). We find that for example, the phase diagram exhibits universal features when the temperature and the stress are appropriately scaled, similar to the universal features of the binding energy and the equation of state (ref. 6).

The model is defined in Section II. We view the solid as a collection of anharmonic springs. If the energy of such a spring is larger than a threshold energy the spring is assumed to fail (ref. 7). Assuming that the relaxation times are short compared to the measurement time, we use equilibrium statistical mechanics to compute the various thermodynamic quantities, such as the strain-stress dependence. The partition function for the anharmonic "springs" defined on percolation clusters is calculated exactly (this model is quite similar to the annealed Ising model on percolation clusters (ref. 8)).

In Section III we present numerical results based on the analytical results of Section II. In particular we determine the phase diagram in the temperature, stress plane. There are two types of transitions: (1) the softening transition corresponding to the thermodynamic instability when the isothermal derivative of the stress with respect to strain is zero; (2) when the network of failed springs percolates the solid becomes brittle. The two transition lines meet at a new type of multicritical point. The two curves have the same slope at the multicritical point. Our concluding remarks are found in Section IV.

II. MODEL

The energy of the "spring" is given by the universal relation discovered by Ferrante et al. Phys. Rev. B 28, 1835 (1983):

$$E = -E_c(1+\eta\varepsilon)\exp(-\eta\varepsilon) \tag{1}$$

where $\varepsilon = (a - a_0)/a_0$ is the strain, η is a parameter controlling the anharmonicity of the spring, and E_C is the cohesive energy.

Assuming that the "springs" fail independently one of another with a probability 1–p, the partition function is:

$$Z = \sum w^B \tag{2}$$

In equation (2) the sum is over all possible configurations of unbroken springs, $w = p/(1-p) = \exp(-\Delta E/T)$, $\Delta E = E - E_0$, E_0 is the threshold energy, and B is the number of unbroken "springs." The summation in equation (2) gives $Z = 1/(1-p)^N$, where N is the number of lattice edges. Then the free energy per lattice edge is:

$$f = -T\ln Z/N = -T\ln\left[1+\exp(-\Delta E/T)\right] \tag{3}$$

The fraction of all edges that have intact springs is equal to p:

$$p = 1/\left[\exp(\Delta E/T)+1\right] \tag{4}$$

The stress σ is obtained by differentiating the free energy with respect to strain:

$$\sigma = \partial f/\partial\varepsilon = E_c p\eta^2\varepsilon\exp(-\eta\varepsilon) \tag{5}$$

The entropy and the specific heat are obtained by differentiating the free energy with respect to the temperature: $s = -\partial f/\partial T$, $c = T\partial s/\partial T$. It is apparent from equations (1) to (5) that this model exhibits universal features when the variables are scaled as follows: E_C/T, $\sigma/E_C\eta$, $\eta\varepsilon$.

There is a thermodynamic instability when $\partial\sigma/\partial\varepsilon = 0$. Physically this instability corresponds to the solid becoming **soft**. In the temperature, strain plane the instability occurs at:

$$1-p = \left(T/E_C\right)(\eta\varepsilon)^{-2}(1-\eta\varepsilon)\exp(\eta\varepsilon) \tag{6}$$

where p is obtained from equations (4) and (1). In the zero temperature limit the instability occurs for: (a) expansion at $\varepsilon\eta = 1$, due to the inflection point (ref. 9) in the energy curve, equation (1); (b) compression at $\varepsilon\eta = -1$, due to the transition from a state of no broken springs if $\varepsilon\eta < -1$ to a state where all springs are broken if $\varepsilon\eta > -1$.

Our model solid undergoes still another transition when the failed springs form an infinite (percolating) cluster, corresponding to a **crumbling** solid. In the case of the FCC lattice the percolation threshold (ref. 10) is:

$$1-p = 0.119 \tag{7}$$

From equations (4) and (7) we determine the location of the crumbling transition:

$$\Delta E/T = -2.00 \tag{8}$$

In the temperature-stress plane, the **crumbling** and **softening** transition lines meet at two multicritical points which to the best of our knowledge were not studied before. At the multicritical points the two transitions lines have the same slope as a consequence of the vanishing of the bulk modulus, $\partial\sigma/\partial\varepsilon = 0$.

III. NUMERICAL RESULTS

The numerical results that follow were obtained from equations (1) to (8). We chose the values of the material dependent parameters E_C/T and η to facilitate the presentation of the qualitative behavior of the various quantities. In figure 1, we show the isothermal dependence of the fraction of unbroken springs p as a function of the strain ε. There is a maximum at equilibrium, zero strain, corresponding to the minimum in energy. Due to the anharmonicity of the spring, the dependence is not symmetrical between the compression ($\varepsilon < 0$) and expansion ($\varepsilon > 0$) regions.

In figure 2 we show the stress-strain relationship. Close enough to the equilibrium the Hooke law applies, i.e., linear dependence $\sigma \approx E_C p \eta^2 \varepsilon$. Because of the anharmonicity built in the energy function, equation (1), there is a marked lack of symmetry between the compression and expansion regimes. The solid becomes soft (thermodynamically unstable) when the stress-strain relation exhibits a minimum under compression and a maximum under expansion. The failure of our model solid under compression may signal the proximity of a transformation to another phase, though the model is too simplistic to incorporate the new phase.

In figures 3 and 4 we show the isothermal variation of the entropy and the isostrain specific heat with the strain. The specific heat shows a Schottky hump (ref. 11) due to the two-state nature of the model: unbroken and broken springs. A second extremum occuring at $\varepsilon = 0$ can be traced back to the minimum in energy at zero strain.

The phase diagram in the strain, temperature plane is shown in figure 5 and in the stress, temperature plain in figure 6. To show the universality feature of the model we use for these two figures the scaled variables T/E_C, $\sigma/E_C\eta$, $\eta\varepsilon$. The crumbling transition line meets the softening transition lines at two multicritical points, one in the compression region and the other in the expansion region. When the threshold energy E_0 is lowered the region where the solid is stable is diminished. Furthermore the anharmonic effect (i.e., lack of symmetry between compression and expansion regions) becomes less important.

While in all the numerical results presented above we set the threshold energy E_0 equal to zero, E_0 can be used to connect this model solid to real solids. It is well known (ref. 12) that the ideal strength (stress value where the solid becomes soft) greatly exceeds that experimentally achieved. The explanation generally proposed is the high defect density (even under zero stress) which limits the value of the strength. For our model solid under zero stress the density of defects is

$$1 - p = 1\Big/\Big[\exp\big((E_0 - E_C)/T\big) + 1\Big] \tag{9}$$

Thus by adjusting E_0 we can reach the defect density of a real solid. The defect density and then E_0 can also be estimated from the slope of the stress versus strain dependence at zero strain.

IV. CONCLUDING REMARK

We plan to extend this work in the following directions: (1) account for correlations between failed springs by using the mapping (ref. 8) between correlated percolation and the Potts model and (2) account for position dependent strains. Miron Kaufman was supported by a NASA-ASEE Summer faculty fellowship.

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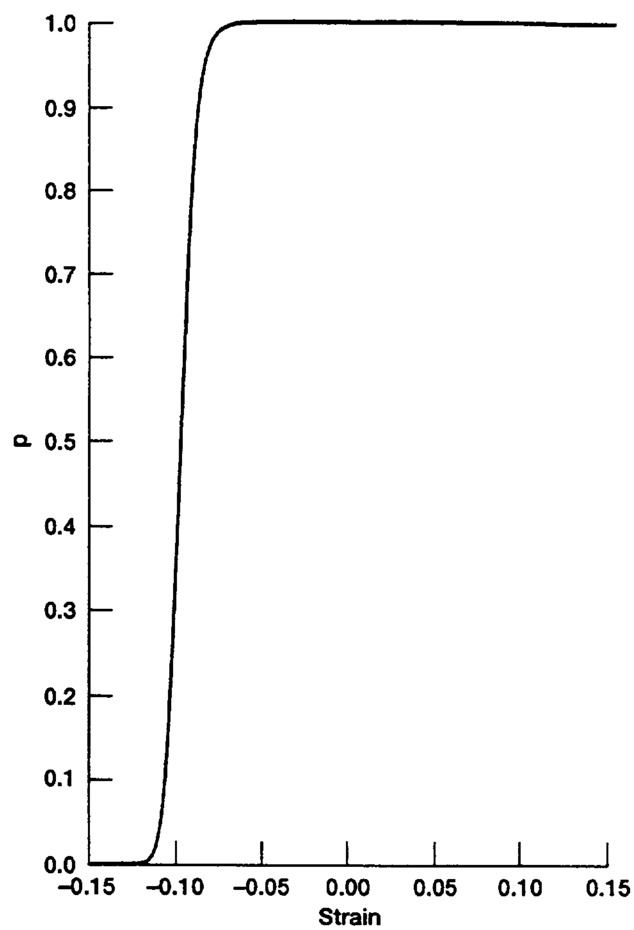

Figure 1.—Fraction of unbroken springs p versus the strain ε, for $\eta = 10$ and $E_c/T = 10$.

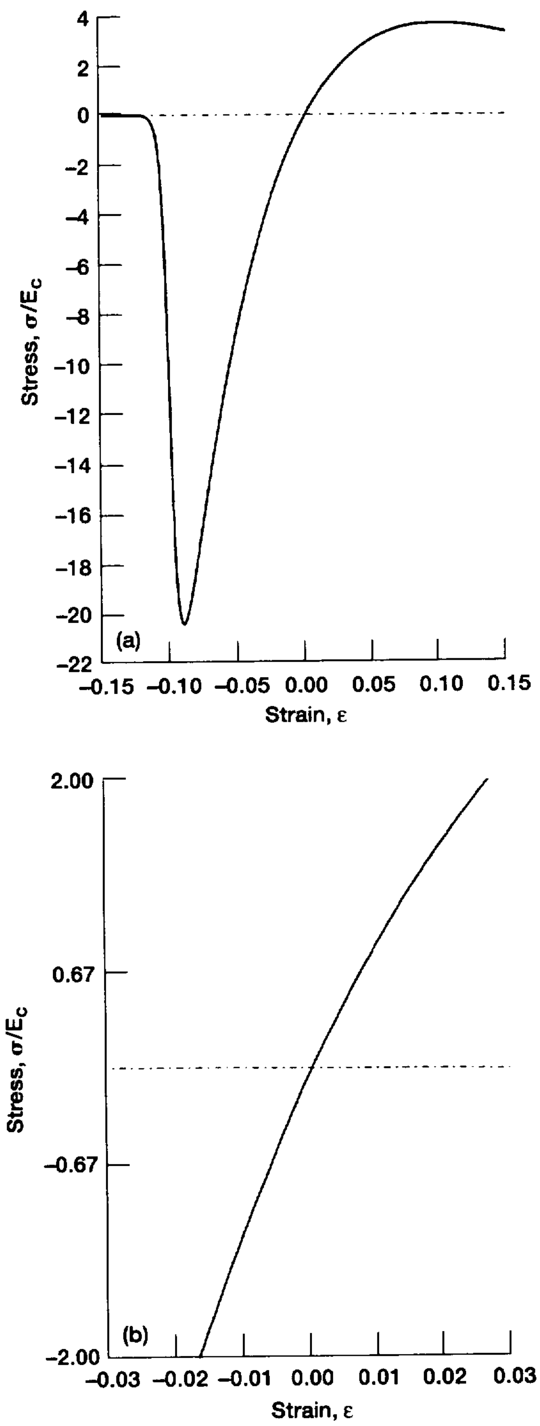

Figure 2.—(a) Stress σ/E_c versus strain ε for $\eta = 10$ and $E_c/T = 10$. (b) Zoom in the small strain region of stress σ versus strain ε, for $\eta = 10$ and $E_c/T = 10$.

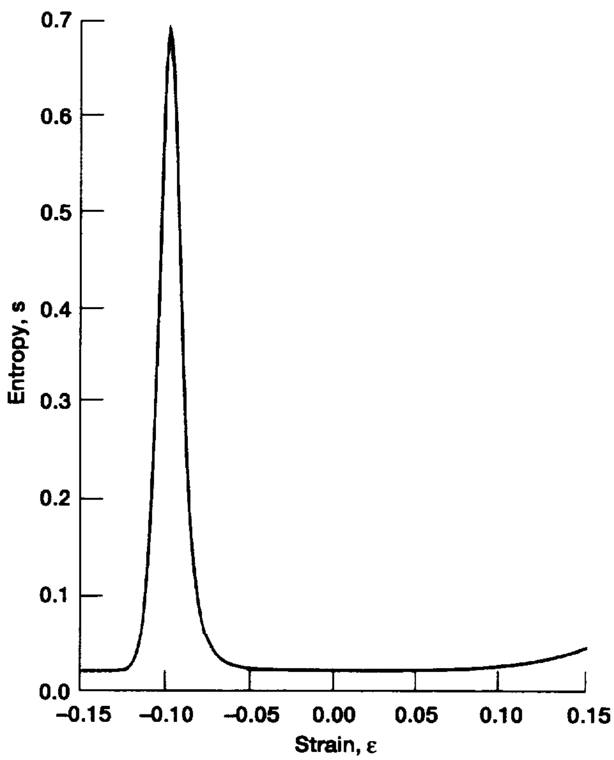

Figure 3.—Entropy s versus strain ε, for η = 10 and E_0/T = 10.

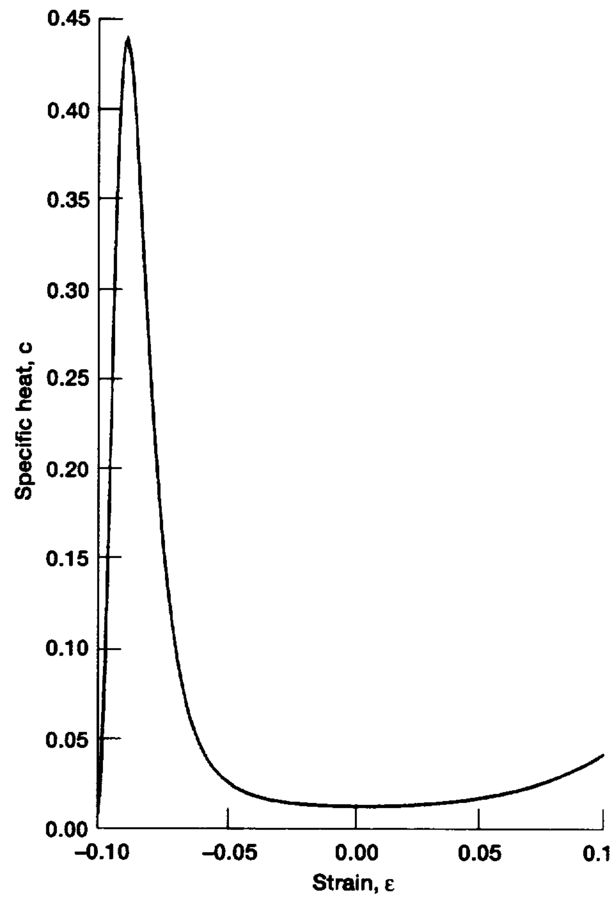

Figure 4.—Isostrain specific heat c versus strain ε, for η = 10 and E_0/T = 10.

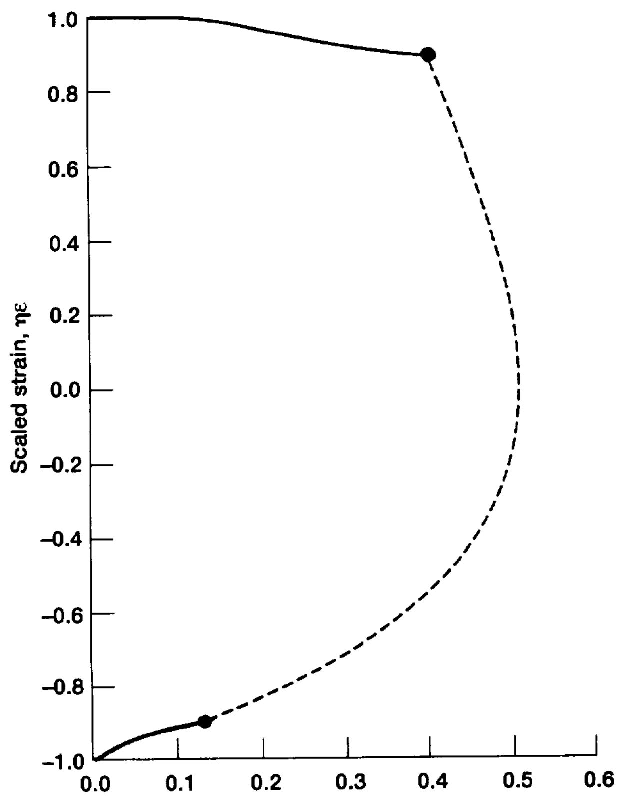

Figure 5.—Phase diagram in the scaled temperature T/E_C, scaled strain $\varepsilon\eta$ plane. Crumbling transitions occur at the dashed line and softening transitions occur at the solid lines.

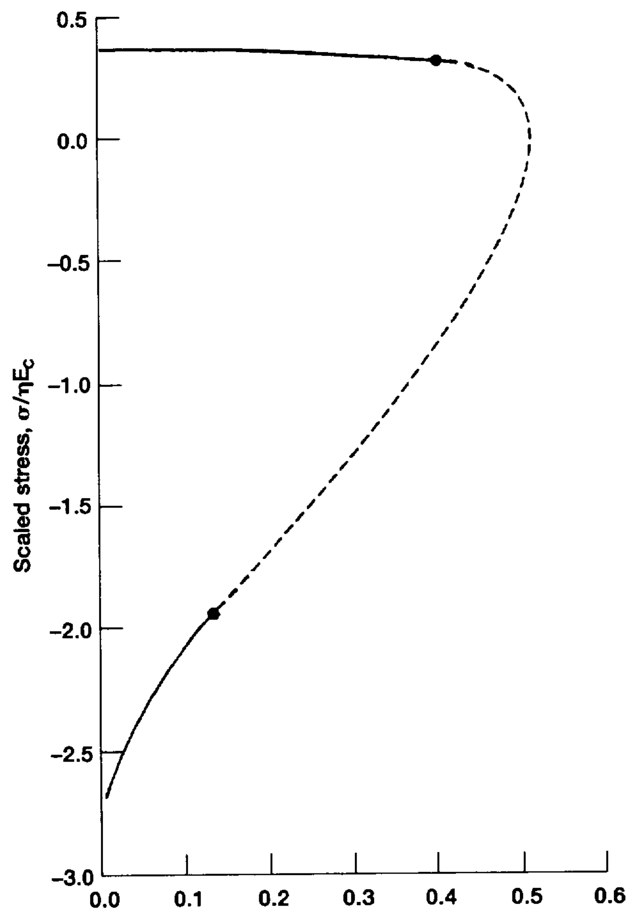

Figure 6.—Phase diagram in the scaled temperature T/E_C, scaled stress $(\sigma/\eta E_C)$ plane. The softening transition lines (solid) intersect tangentially the crumbling transition line (dashed) at two multicritical points.

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